Undec-10-ynoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C17H26O2/c1-4-7-8-9-10-11-12-13-15-17(18)19-16(6-3)14-5-2/h1,16H,6-13,15
InchiKey: YMISBVOGWGPTQT-UHFFFAOYSA-N
Formula: C17H26O2
SMILES: C#CCCCCCCCCC(=O)OC(C#CC)CC
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	281.77	kJ/mol	Joback Method
hf	-80.09	kJ/mol	Joback Method
hfus	45.15	kJ/mol	Joback Method
hvap	64.21	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.086		Crippen Method
mcvol	240.630	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
rinpol	1876.00		NIST Webbook
rinpol	1876.00		NIST Webbook
tb	663.33	K	Joback Method
tc	855.83	K	Joback Method
tf	491.58	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.32	J/mol×K	663.33	Joback Method
cpg	660.65	J/mol×K	695.41	Joback Method
cpg	677.11	J/mol×K	727.50	Joback Method
cpg	692.74	J/mol×K	759.58	Joback Method
cpg	707.55	J/mol×K	791.67	Joback Method
cpg	721.58	J/mol×K	823.75	Joback Method
cpg	734.84	J/mol×K	855.83	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406964&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume